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13. ABSTRACT *(Maximum 200 words)*

A pulse propagation method for tracing the path of a short wavelength signal through a medium with varying index of refraction and over complex, reflecting terrain has been developed. The method is completely Eulerian and does not use any markers that can become sparse as the signal spreads in the lateral direction. On the other hand, unlike conventional Eulerian wave equation methods, the signal does not suffer degradation due to numerical error such as diffusion, even though the wavelength is of the order of a grid cell and the signal can propagate over arbitrarily long distances. During the contract period, it has been demonstrated, both theoretically and numerically, that there are no interaction effects when signals pass through each other, even after a large number of interactions. This is true of the actual linear wave equation that is being simulated, but had to be shown for our numerical method, which has a strong nonlinear component.

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Final Report

A Local Parabolic Method for
Long Distance Wave Propagation

Contract No. **FA9550-04-C-0033**

Period: **4/12/04-4/11/05**

Principal Investigator: John Steinhoff

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1. Introduction

1.1 Computation of Propagating Pulses

The main requirement of the **Local Parabolic Method** (LPM) development is a method to compute thin propagating wave equation pulses that do not spread due to numerical effects.

(This part of the research will, by itself, be important for computing long distance propagation of pulses in the time domain.)

A general method is described to efficiently simulate these wave equation pulses, in Eulerian computations on fixed, coarse grids. The method, "Lattice Confinement", involves treating the features as solitary waves that obey nonlinear, difference equations, which are different from Taylor expansion– based discrete approximations to the governing, partial differential equations (pde's). These equations are rotationally invariant generalizations to multiple dimensions of 1-D discontinuity confinement schemes. The method is a generalization of an earlier method, "Vorticity Confinement" [1], which was successful in efficiently treating thin, vortical regions.

For long distance propagation of pulses, direct discretization and solution of the governing partial differential equations (pde's) using conventional Eulerian Taylor expansion –based numerical methods to resolve the thin features can be prohibitively expensive. Even adaptive unstructured grid methods are very expensive and complex for general problems with many small-scale, time-dependent features. Fortunately, the details of the internal structure of these small features are often not as important as integral quantities. The quantities of importance for our purpose are the centroid motion and total integrated amplitude at each point along the pulse surface. The main issue in computing these cases is that conventional pde-based methods require a relatively large number of grid cells (4-8) across each small dimension to treat a feature, such as a wave equation pulse. Even then, the details of the internal structure will be mainly determined by the discrete numerics, and not the physics of the pde. Also, numerical discretization errors will still build up over long distances, causing, for example, large, unphysical spreading.

This leads us to the idea of simulating or "modeling " the thin features directly on the grid with *difference* equations, rather than attempting to accurately discretize the pde's for them using *finite difference* approximations. The idea of modeling, or solving for small-scale features directly on the grid without using smoothness assumptions or Taylor expansions, i.e., as "weak solutions", goes back to work of Lax and others [2], but was applied mostly to shocks. Shocks, however, effectively, "capture themselves" because they have converging characteristics. Harten [3] did treat contact discontinuities in this way, which do not have converging characteristics, but for 1-D compressible flow.

First, the Lattice Confinement method will be reviewed for wave equation pulses. Some results will then be presented for short scalar pulses obeying the wave equation (with Lattice Confinement). Previous results [4] for a 2-D pulse reflecting from planar

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surfaces will be shown, then 3-D results for a pulse reflecting from complex objects (a missile and an aircraft). This missile case will involve multiple, curvilinear grids.

1.2 Main Features of Lattice Confinement
(Parts of this section are related to Ref. [4])

The main idea is to treat thin features as nonlinear solitary waves that "live" directly on the grid lattice, spread over only a few cells. The internal structure is determined by the discrete lattice equations. The total amplitude, centroid and (in a future extension), a few moments, however, are determined by the physics. These quantities are transported across the grid with essentially no numerical errors (for constant slowness). For smoothly varying slowness, small discretization effects will occur, based on the longer length scale of the slowness variation, but not based on the shorter length scale of the pulse..

Essentially, these discrete equations define a simple, implicit model which obeys a "fast" dynamics, relaxing to an asymptotic, propagating state in a few time steps. In this way we can simulate the most important physical effects of the small scales, which cannot be accurately computed by just discretizing the governing pde's on the given grid. These effects can be, for example, that thin wave equation pulses propagate over long distances without spreading in a smooth, slowly varying external field, and that they can merge or reflect, respectively, and thus change topology.

1.2.1 Stationary Case

The formulation presented here is related to that presented in [5] in 1-D. First a stationary pulse is discussed, requiring only an iteration of the Lattice Confinement terms, so that the simple asymptotic form can be seen. Advection, in general, will change this form somewhat. However, in the limit of small advection time step, or if a number of these "Confinement" steps are taken for each convection step, then the following form should result. The same is true for the wave equations. Results very close to these are also found with advection steps that are not small; these are shown in Ref. [5].

We start with an iteration sequence for a single-signed scalar, ϕ :

$$\partial_t \phi = \frac{h^2}{\Delta t} \nabla^2 \left[\mu\phi - \varepsilon\Phi \right]$$

or

$$\phi^{n+1} = \phi^n + h^2 \nabla^2 (\mu\phi^n - \varepsilon\Phi^n) \qquad (1.1)$$

where Φ is a nonlinear function of ϕ (given below) and μ is a diffusion coefficient that can include numerical effects in a convection or wave equation solution (we assume physical diffusion is much smaller). The discretized grid cell size is h and time step, Δt. For the last term, ε is a numerical coefficient that, together with μ, controls the size and time scales of the confined features. For this reason, we refer to the two terms in the brackets as "Confinement terms".

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The two (positive) parameters, ε and μ, are determined by the two small scales of the computation, h and Δt, since we want the small features to relax to their solitary wave shape in a small number of time steps and to have a support of a small number of grid cells. Thus, even though h may be small, the Laplacian will be large and the total effect also large.

For the propagating pulse problem, it is assumed that the slowness field is propagating is slowly varying compared to these scales (this is required if the grid cell size and time step are to resolve the pde's governing this outer flow). Relaxation of this assumption will be studied in the proposed effort. We then have a two-scale problem with the thin structure obeying a "fast" dynamics:

$$\mu\phi - \varepsilon\Phi \approx 0 .$$

With propagation in a "slow", smooth external field, this relation is still approximately satisfied, as verified by computations and heuristic arguments [4].

There are many possibilities for Φ. A simple class is

$$\Phi^n = \left[\frac{\sum_l C_l (\widetilde{\phi}^n)^{-\rho}}{\sum_l C_l} \right]^{-1/\rho} \qquad (1.2)$$

$$\widetilde{\phi}^n = |\phi|^n + \delta .$$

The above sum is over a set of grid nodes near and including the node where Φ is computed. The absolute value is taken and δ, a small positive constant ($\sim 10^{-8}$), is added to prevent problems due to finite precision. The coefficients, C_l, can depend on l, but good results for many cases are obtained by simply setting them as well as ρ to 1. Then, Φ is the harmonic mean of ϕ on the local stencil. Other forms could also be used, with $\rho > 1$. $\rho = \infty$ corresponds to the minimum of the absolute value: for 2-D and 3-D applications discontinuous operators such as "min" will not result in as smooth distributions as continuous ones, and we use only $\rho = 1$ or $\rho = 2$.

An important feature of Lattice Confinement is that all terms are homogeneous of degree 1 in Eqn. 1.1 (as they are in the wave equation). This is necessary because the Lattice Confinement terms should not depend on the scale of the quantity being confined. Another important point is that wavelengths longer than the thin features that are to be confined must have a negative diffusive behavior, so that the features remain confined, that is stable to perturbations against spreading. This means that Φ must be nonlinear: It is easy to show by Von Neumann analysis that a linear combination of terms, for example of second and fourth order, cannot lead to a stable Confinement for any finite range of

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coefficients: any wavelength that exhibits negative diffusion would then eventually diverge.

1.2.2 Wave Equation Formulation

We start with the 1-D scalar wave equation with constant wave speed, c, for simplicity. As in scalar convection, we add an additional term to control the shape of a short pulse:

$$\partial_t^2 \phi = c^2 \partial_x^2 \phi + \partial_x^2 \psi$$

or, using a simple time discretization,

$$\phi^{n+1} - 2\phi^n + \phi^{n-1} = c^2 \Delta t \partial_x^2 \phi + \Delta t \partial_x^2 \psi \qquad (1.3)$$

It was seen in Ref. [6] that the addition of "Lattice Confinement" terms in the form of second derivatives of a function that has finite support do not change the propagating speed (nor the total amplitude) of a propagating, confined pulse. The same is true for the wave equation, if an additional time derivative is applied. This means, of course, that they do not change the motion of the centroid of an isolated pulse.

The main constraint on the Confinement term, ψ, is that it force an initial isolated, propagating compact pulse with a single maximum to remain compact and not develop any additional maxima. We use:

$$\psi^n = \mu \delta_n \phi^n - \varepsilon \delta_n \Phi^n (\phi^n) \qquad (1.4)$$

In this term Φ has the form given by Eqn. (1.2) in terms of its argument. We have defined

$$\delta_n f^n = f^n - f^{n-1}$$

Results will be given in Section 4 using this form.

An important feature of the method is that the waves do not suffer a "phase shift" when they pass through each other. This is obvious for the equation we want to simulate – the linear wave equation. However, the Confinement term is nonlinear. Such a phase shift would show up as a kink in two waves in 2 or 3 dimensions that are passing through each other, and can be studied in detail in 1-D. It turns out that there is no kink, to plottable accuracy, as can be seen in the plotted scattering results in Sec. 4.1. Results for the centroid trajectories for 2 pulse passing through each other in 1-D are presented in Fig. 1. There, the computed centroids are plotted as solid lines and the exact as dashed (the periodic boundary conditions can be seen in the former). It can be seen that there is no phase shift to plottable accuracy. This lack of nonlinear interaction persists, according to our study, in the limit of small time step (2 orders of magnitude smaller that that of Fig. 1), even though $O(10^2)$ confinement corrections were applied as the pulses were

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overlapping. We attribute this to the existence of another conserved variable, similar to total energy. This computation was done by Nick Lynn of University of Tennessee Space Institute (UTSI).

One other important use of Lattice Confinement for the wave equation involves cases with multiple grids with grid interfaces. If only the discretized wave equation is used, with no Confinement, reflections result from small numerical errors at the grid interfaces, unless special care is taken. Lattice Confinement completely overcomes this problem and the (single) pulse propagates across the interface with no reflections.

Some of the advantages of using direct difference equations instead of pde's for a related problem can be found in Ref. [7]. There, a very efficient formulation is derived for the Helmholtz equation by minimizing the L_2 norm of the error of waves propagating with fixed $\left| \vec{k} \right|$.

1.3 Vector Potential Formulation

In a recent promising development in our wave equation research, we have implemented a vector potential, $\vec{A}$, as the basic variable, instead of a scalar representing the $\vec{E}$ and $\vec{B}$ fields. If sufficient time is available, this formulation will be investigated in detail.

Even though there is no direct effect of this alternative formulation in classical electromagnetics, there is a major advantage in the computation of pulse solutions. This is because, for a thin pulse, $\vec{E}$ and $\vec{B}$ only have a small region of support, but $\vec{A}$ extends throughout the field. The $\vec{E}$ and $\vec{B}$ representation of the pulse is a spread delta function across the width, but the $\vec{A}$ representation is a step function. As a result, it is much easier to capture the pulse by operating on $\vec{A}$, since it is topologically "trapped" by this field. The argument is exactly the same as in Vorticity Confinement, where thin vortical regions $(\vec{\omega})$ are trapped in a velocity field, $\vec{q}$, extending throughout space. (This is also related to the trapping of defects in other field theories). The resulting confinement terms are exactly the same in the two cases, with $\vec{A}$ corresponding to $\vec{q}$ and $\vec{B}$ corresponding to $\vec{\omega}$.

The formulation is
$$\vec{B} = \vec{\nabla} \times \vec{A}$$
$$\delta_t^2 \vec{A} = c^2 \nabla_D^2 \vec{A} + \mu \delta_t \nabla_D^2 \vec{A} + \varepsilon \delta_t \vec{\nabla}_D \times \vec{b}$$
where $\vec{b}$ is a local harmonic mean of $\vec{B}$ at each grid point:
$$\vec{b} = \frac{\vec{B}}{|\vec{B}|} \left[\sum_\ell \frac{|\vec{B}_\ell|^{-1}}{N} \right]^{-1}$$
where δ_t and ∇_D denote discrete operators and Eqn. 1.2 was used with a sum over N neighboring points, labeled ℓ. In the formulation the Coulomb gauge was used so that a

scalar potential does not appear in the equation for $\vec{B}$. Also, $\vec{\nabla} \cdot \vec{A} = 0$ is then enforced. This is also directly analogous to the incompressibility condition, $\nabla \cdot \vec{q} = 0$.

2. Objectives

Develop "pulse Capturing" method to generate approximate short wavelength solution which is useful by itself for computing long distance amplitudes and which will provide a coordinate system for the locally parabolic propagation method.

3. Status of effort

Have developed a pulse propagation method for tracing the path of a short wavelength signal through a medium with varying index of refraction and over complex, reflecting terrain. The method is completely Eulerian and does not use any markers that can become sparse as the signal spreads in the lateral direction. On the other hand, unlike conventional Eulerian wave equation methods, the signal does not suffer degradation due to numerical error such as diffusion, even though the wavelength is of the order of a grid cell and the signal can propagate over arbitrarily long distances. During the contract period, it has been demonstrated, both theoretically and numerically, that there are no interaction effects when signals pass through each other, even after a large number of interactions. This is true of the actual linear wave equation that is being simulated, but had to be shown for our numerical method, which has a strong nonlinear component. Progress has also been made in developing a reflecting formulation that can treat complex terrain. To be feasible for realistic cases, this treatment cannot use surface-conforming computational grids, but must be able to use a simple representation where the surface is "immersed" in a uniform Cartesian grid, with no requirements for complex logic involving the geometry of the "cut" grid cells.

4. Results

4.1 Prior to 4/04

Lattice Confinement was added to the linear wave equation with simple, second order central discretization. A uniform Cartesian grid was used with reflection on the walls of a square region, in 2-D as well as 3-D. In certain cases, it is well known that a "tail" will develop behind a 2-D wave front, while the front remains sharp (if it is initially sharp). In the 2-D computation with Confinement we can keep a sharp pulse and suppress the tail. This tail is smooth and could, if desired, be computed using standard CFD on the grid. The goal, however, was to show that a pulse can propagate over long distances with Lattice Confinement. The same long distance propagation was observed in 3-D where there were genuine pulse solutions.

4.1.1 Reflection from Planar Surface

In Fig.2 2-D results are presented for a 128x128 cell grid. It can be seen that there is no perceptible diffusion of the pulse, even after many reflections. These results were also presented in Ref. [5].

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4.1.2 Scattering from Missile

The first computation involved a planar scalar wave impinging on the nose of a missile. The plane of the wave is parallel to the longitudinal axis of the missile. The magnitude of the scalar is presented in planes parallel (i.e., the symmetry plane) and perpendicular to the longitudinal axis of the missile, and on the surface of the missile body. Figures 3 and 4 depict the intensity of the planar wave before, during, and after reflection from the missile surface in the nose area from the side and from the front, respectively.

The second computation involved the aft-end of the missile. Figure 5 depicts the same sequence, but in the fin area, as seen from the rear. The third computation involved the entire missile. Figure 6 depicts a pulse reflecting from the nose area at 45°, in the symmetry plane, as seen from the side.

Figure 7 depicts part of the overlapping computational grid. The confinement method has been generalized to curvilinear grids for this case. Confinement also prevents reflections from the grid interface regions.

All of the missile results involve a pulse confined to about 3 grid cells except in the fine grid region very near the surface. There, the method reverts to standard CFD. Also, it can be seen in Fig.5 that, unlike in geometrical optics, there is a diffracted component. This will most likely represent a diffracting pulse corresponding to the width of the computational one. We should be able to make corrections to the diffracted intensity to simulate pulses of other widths. This would result in a very general method able to treat diffraction to first order (in this short pulse limit).

4.1.3 Scattering from Aircraft

Next, results of confinement are presented for scattering from an aircraft shape. Here, a uniform Cartesian grid was used with a special treatment of the surface boundary conditions. A level set description of the body was used, which was early derived from a surface definition "STL" file. The contours of scalar intensity are presented in the cross plane depicted in Fig. 8. With these boundary conditions, it can be seen that scattering from very complex shapes can easily be computed. In Fig. 9, contours of the scalar magnitude representing the electromagnetic field are shown for three different times.

The last results involve the new vector potential computation. There, a single contour can be used to represent each part of the wave since the potential extends throughout the field and has a definite range of values within the pulse. Preliminary results are depicted in Fig. 10 for two times. Further work is progressing on the new technique.

4.2 Contract Period

4.2.1 Cahn-Hilliard Equation

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Based on comments by Fernando Reitich and Bill Rider, a connection between Cahn-Hilliard (CH) – type equations and our discrete convection equation (eqn.1.1) was investigated. This commonality includes the same linear convection terms and the appearance of a Laplacian in front of the non-linear term. This commonality is not surprising since the CH equation was originally proposed as a phenomenological description for the dynamics of thin fluid interfaces in otherwise smooth flows, and our equation describes thin pulses propagating in otherwise smooth fields. To derive the continuum limit of our equation, a parameter limit was derived such that the pulses were spread over an arbitrarily large number of grid cells. (Though the equations are similar, the resulting non-linear term is not exactly the same as in the commonly used form of the CH equation). The derivation is described in Fig. 11.

4.2.2 Suppression of Nonlinearity Effects in Pulse Interaction

As described in Sec. 1.3, to represent intersecting wave equation solutions, when pulses pass through each other, there must be no amplitude exchange or phase shift. Otherwise, the actual wave equation being studied could not be accurately simulated, since it is linear. However, a nonlinear term is required in the discrete equation in order to create a solitary wave representation of the pulse which will be non-diffusing. A nonlinear term in the wave equation, of course, usually results in interactions between intersecting pulses, including the above effects. As explained in Sec. 4.1, it had been shown numerically, to plottable accuracy, that for our formulation these effects are absent. A new analytic result was obtained that shows that, for the formulation used, this interaction effect vanishes in the Born approximation. This vanishing is due to the fact that both the Laplacian and the time derivative operator operate on the nonlinear term. This derivation is described in Fig. 12.

4.2.3 Reflection from Complex Terrain

Physical terrain consists, of course, of many irregularities. For short pulses, or high frequencies, these irregularities can be larger than the wavelengths. This seems to preclude attempting to achieve high accuracy after reflection, except for special cases involving very smooth surfaces. For this reason, one of the main reasons for the use of higher order discretizations in conventional treatments of long distance propagation may not involve increasing accuracy after reflection, but to attempt to reduce numerical diffusion in the propagation. Since we do not have this diffusion problem, and we are treating complex, irregular terrain, we feel that we can use more efficient, lower order discretizations with no loss of accuracy. We can then implement a very effective method for treating reflections (and absorption). This method does not require complex, surface-fitted grids, but allows the terrain surface to be simply "immersed" in a uniform Cartesian grid. This method employs a "level set" representation of the surface and can easily accommodate very complex topography with little computational penalty. A picture of the representation for a simple object is shown if Fig. 13. During the computation, as explained in Ref. [4], each time step, the wave amplitude is simply set to zero inside the surface. The nonlinear "confinement" term keeps the surface definition sharp. However,

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since the term steepens the pulse only in the normal direction, the pulse surface is treated as smooth in the tangential direction. As a result, grid effects such as "staircase" are avoided and an accurate reflection is obtained. The scattering results presented in Sec. 4.1 used this method.

New results have been obtained with this method for scattering of pulses from 2-D and 3-D terrain. The 2-D results, including some diffraction effects, are presented in Fig. 14. (Amplitude contours are shown in this and other plots depicting pulse scattering). Reflection from a 3-D wedge, depicted in Fig. 15, is shown in the short wave limit (with no diffraction) in Fig. 16.

4.2.4 Computation of Eikonal Phases (Frequency Domain)

Even though the pulse representation in the short pulse limit will be of direct use in computing amplitudes and arrival times in that limit, the computation of diffraction and frequency domain amplitudes will also be important.

The first step towards this goal is to use the pulse arrival time at each grid node to determine the Eikonal phase, for each pulse arrival. Preliminary results for scattering from a complex terrain are shown (as time contours) in Fig. 17 for first arrival times, including a possible use for computing diffraction. In Fig. 18, the direct diffracted field is suppressed, but both first and second arrival times are displayed. Initial results for a simpler case with two sources and no scattering are shown in Sec. 4.1.

5. Personnel Supported

The following personnel were partially supported:
Dr. John Steinhoff (US citizen)
Dr. Lesong Wang
Dr. Yonghu Wenren (US citizen)

6. Publications

"Computation of Short Wave Equation Pulses using Non-linear Solitary Waves", M. Fan, L. Wang and J. Steinhoff, *Computer Modeling of Engineering and Sciences*, vol. 5, No. 4, 2004. (Included as Appendix I)

7. Interactions

a) Participations/presentations
- Gave talk on Wave Confinement at the AFOSR contractor's workshop in San Antonio in January.
- Gave seminar on Wave Confinement at the math department of Brown University in February at the invitation of David Gottlieb. David seemed very interested in the property of the formulation that the pulses could pass through each other with no phase shift or change in total amplitude.
- Invited by Fernando Reitich and gave seminar on Oct. 7 at the math department of the University of Minnesota. Fernando has similar interests to David Gottlieb.

b) Advisory functions

Served on the review panel for the Army High Performance Computing Center at the University of Minneapolis, Aug. 16, 17 and 18, held at the center. Reviewed and judged status and quality of projects they are funding involving use of the computer. Principal individual - professor Kumar Tamma, director.

c) Transitions
none, yet.

8. New discoveries

Interaction - free nonlinear solitary waves

9. Honors/awards

10. References

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[4] Steinhoff, J., Dietz, W., Haas, S., Xiao, M., Lynn, N., Fan, M., "Simulating Small Scale Features in Fluid Dynamics and Acoustics as Nonlinear Solitary Waves", *AIAA Conference,* Reno, Nevada, Jan. 6-9, 2003

[5]Fan, M., Wang, L., and Steinhoff, J., "Computation of Short Wave Equation Pulses Using Nonlinear Solitary Waves", to be published in *Computer Modeling in Engineering & Sciences, January, 2004.*

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[7] Caruthers, J., Steinhoff, J., Engels, R., "An Optimal Finite Difference Representation for a Class of Linear PDE's with Application to The Helmholtz Equation" , *Journal of Computational Acoustic*, Vol.7, No.4, 1999, pp.245-252.

11. Figures
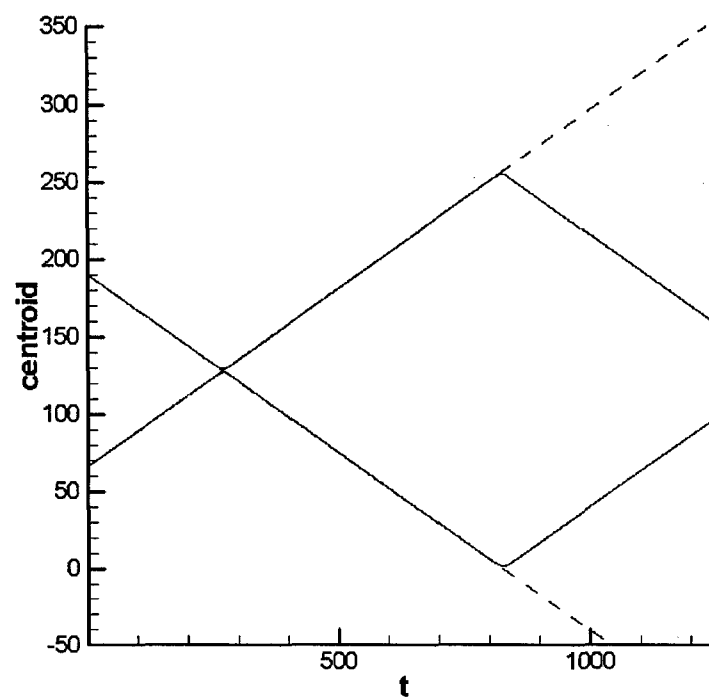
Figure 1. Comparison of Computed Centroid of Pulses with Exact Solution
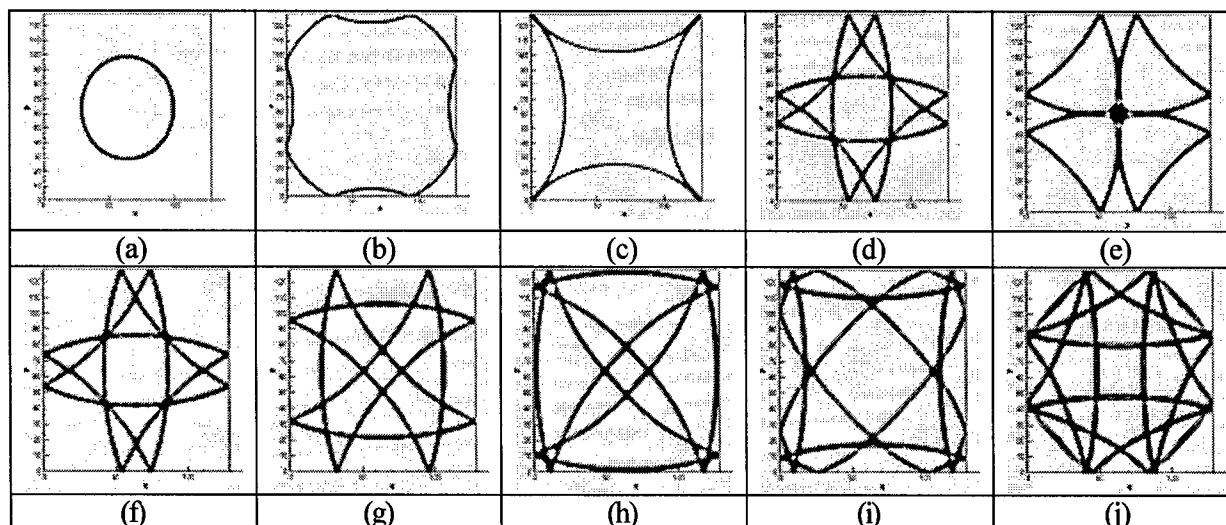
Figure 2.a~j 2D convex wave propagation
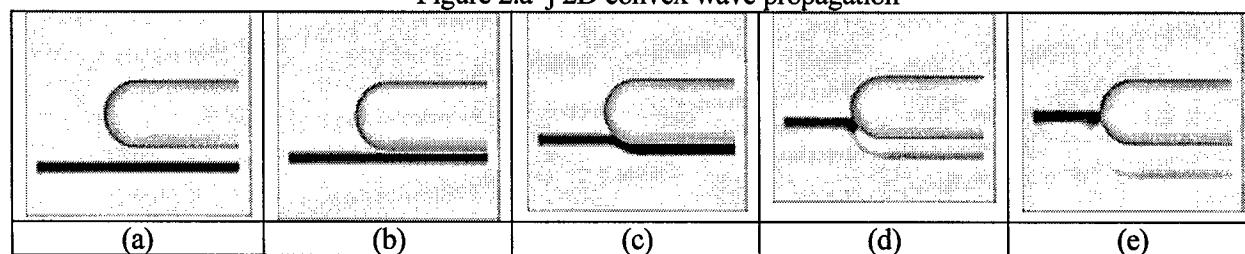
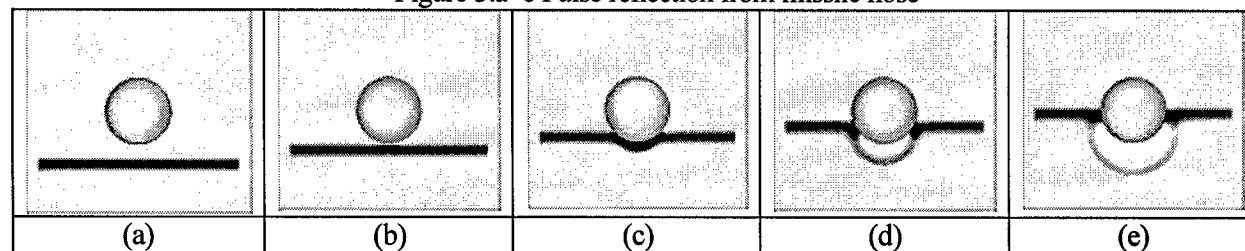

Figure 3.a~e Pulse reflection from missile nose

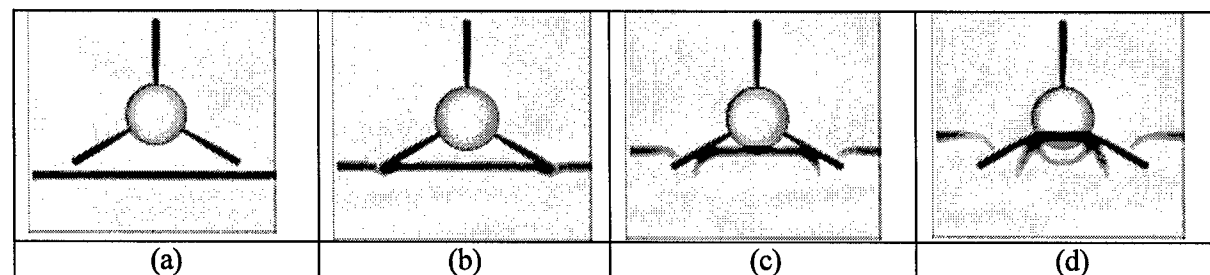Figure 4.a~e Pulse reflection from missile nose
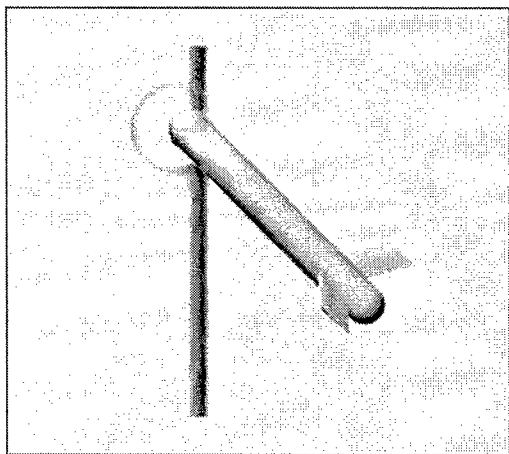

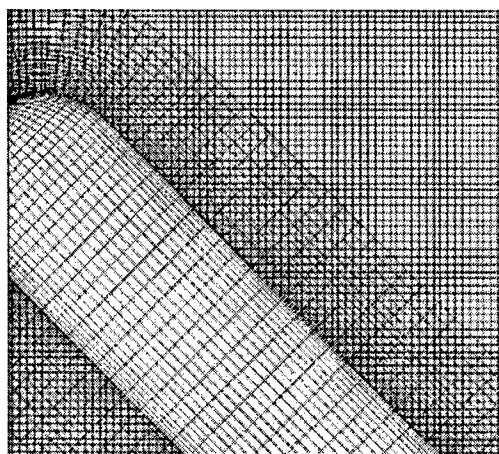Figure 5.a~d Pulse reflection from missile fins

Figure 6. Pulse reflection from missile
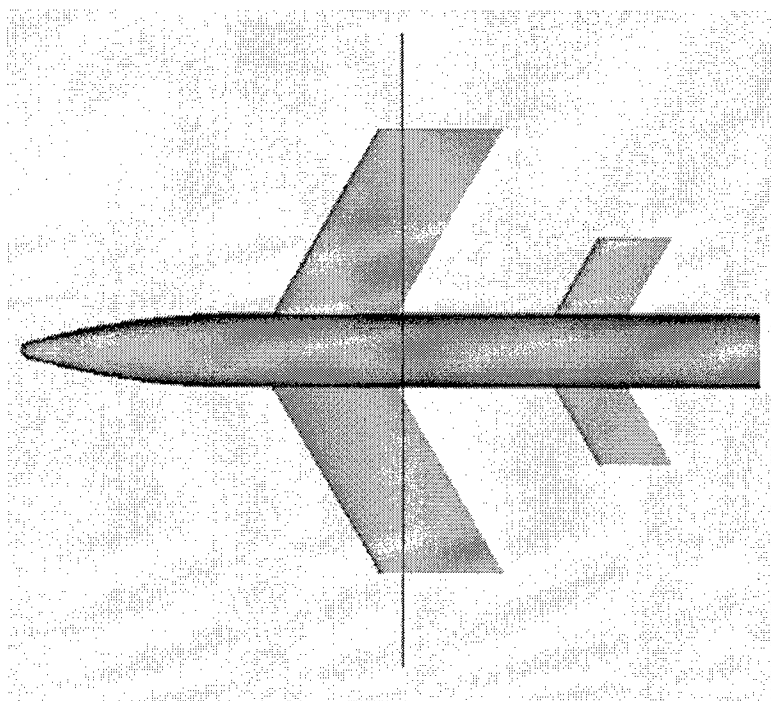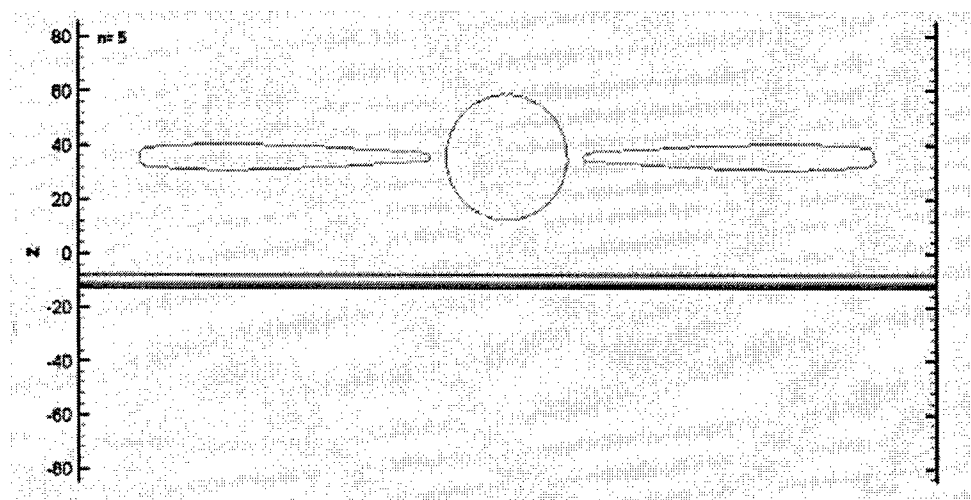

Figure 7. Detail of Missile Grid/
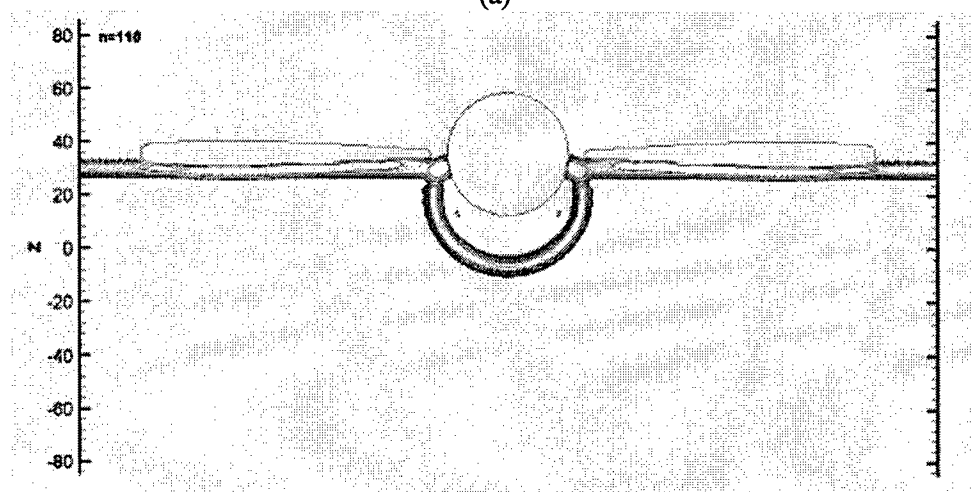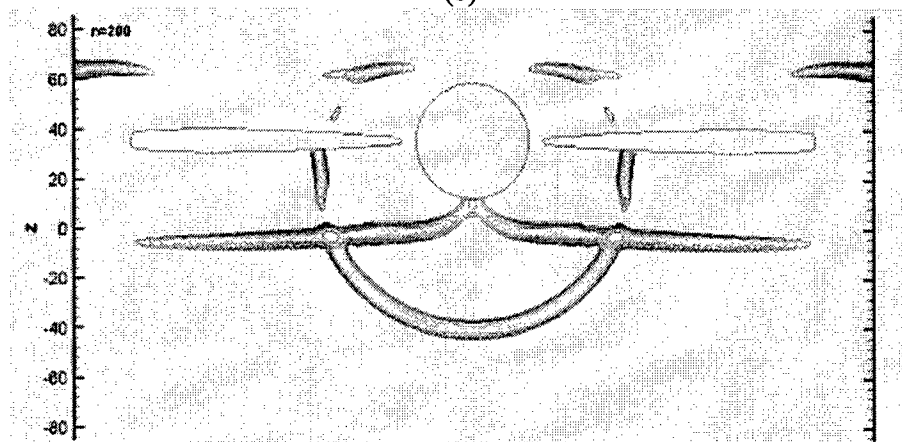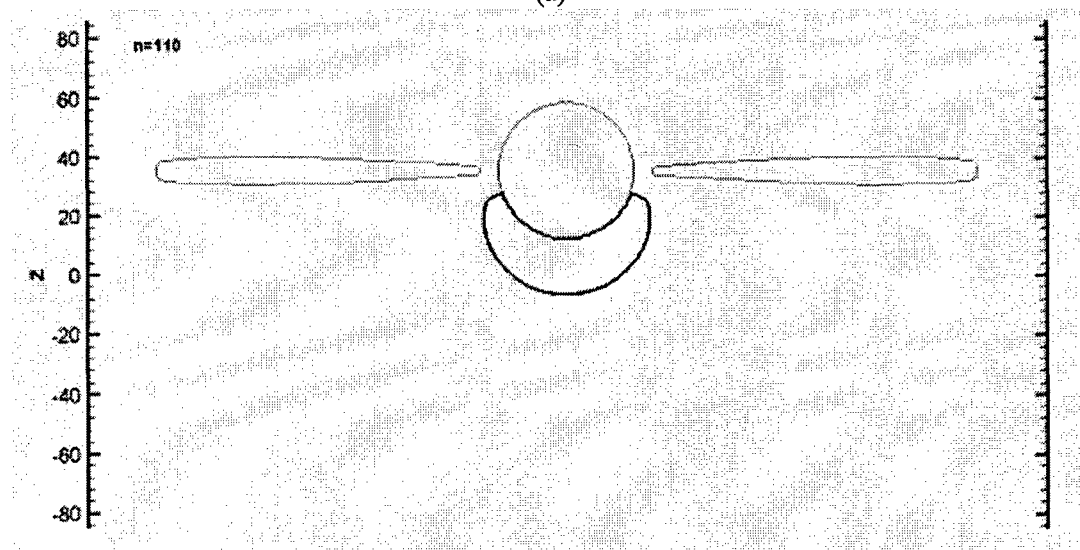Cartesian Grid Overlap Region

Figure 8. Aircraft Configuration

(a)

(b)

(c)

Figure 9.a~c Contour levels (from one third of the maximum to maximum level) of the scalar with vorticity confinement at different time steps (CFL $\approx$ 0.4).
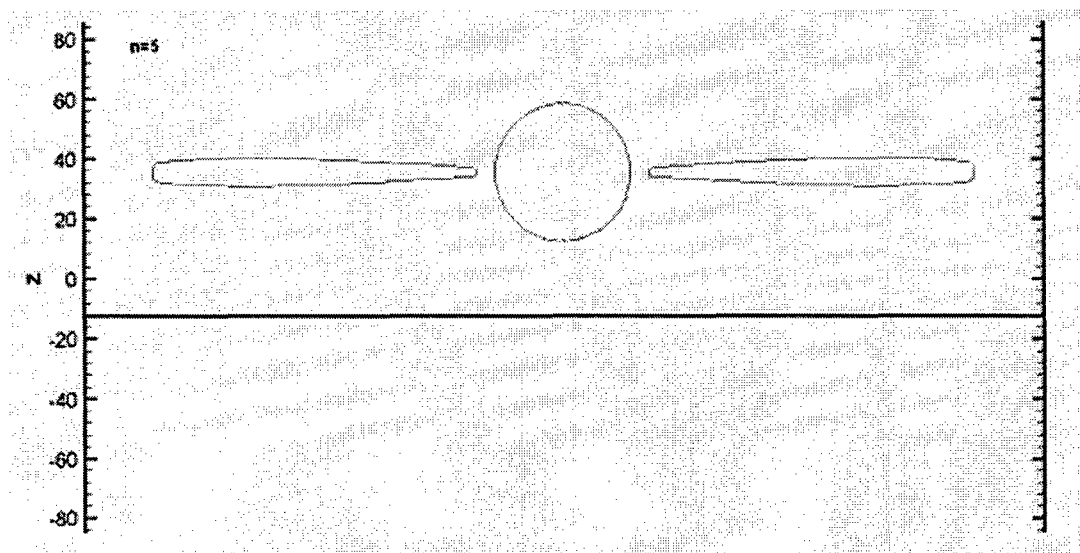
(a)

(b)

Figure 10.a~b Contour line (maximum level) of the vector potential magnitude at different time steps (CFL $\approx$ 0.4).

PDE Limit, $\Delta t, h \to 0$

Taylor Expansion

Cahn Hilliard Equation

$$\mu^* = \mu/\Delta t, \qquad \varepsilon^* = \varepsilon/\Delta t$$

$$\varepsilon^* = \mu^* + O(h^2)$$

$$\tilde{\mu} = \mu^*/h^2$$

$$\alpha = \varepsilon^*/\mu*$$

$$(1+\alpha) = -\gamma h$$

$$\gamma \sim O(1)$$

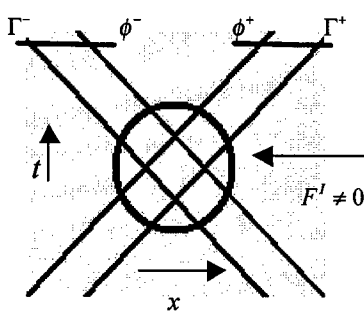$$\partial_t u_j = \frac{c(u_{j+1} - u_{j-1})}{2h} + \frac{\mu^*}{h^2}\delta_j^2(u_j + \alpha F_j)$$

$$F_j = \frac{3}{u_{j-1}^{-1} + u_j^{-1} + u_{j+1}^{-1}}$$

$$\partial_t u + c\partial_x u = \mu^*(1+\alpha)\partial_x^2 u + h^2\partial_x^2 \frac{\mu^*\alpha}{3}\left(\partial_x^4 u - \frac{2(\partial_x u)^2}{u}\right)$$

$$\partial_t u + c\partial_x u = \frac{\tilde{\mu}}{3}\partial_x^2\left(-\gamma u - \partial_x^2 u + \frac{2(\partial_x u)^2}{u}\right)$$

Figure 11

Born Approximation

$$\partial_t^2 \phi = c^2 \partial_x^2 \phi + \partial_t \partial_x^2 F$$

$$F = F\left(\phi^+ + \phi^- + \phi^I\right)$$

$$= F\left(\phi^+\right) + F\left(\phi^-\right) + F^I$$

Change in $\phi \equiv \phi^I$

$$(\partial_t^2 - c^2 \partial_x^2)\phi^I = \partial_t \partial_x^2 F^I$$

After interaction have integrals for change
in A and $< x >$

$$\delta A_{\pm}^I = \int_{\Gamma^{\pm}} dx \phi^I = 0$$

$$\delta \langle x \rangle_{\Gamma}^{\pm} = \left(\int_{\Gamma^{\pm}} dx x \phi^I \right) \Big/ A^{\pm} = 0$$

These vanish by Gauss's Theorem because of
differentials in front of F^I

Figure 12

"Immersed" Boundary
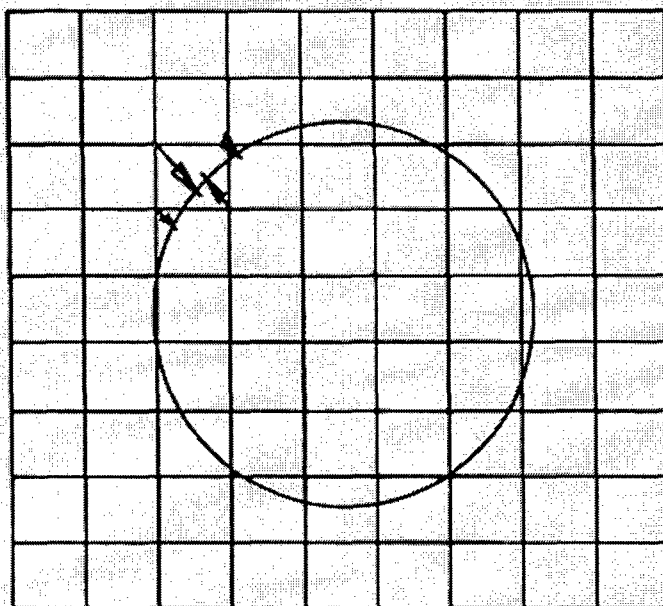
SURFACE DEFINITION

For Approximate B.C.'s

F Function

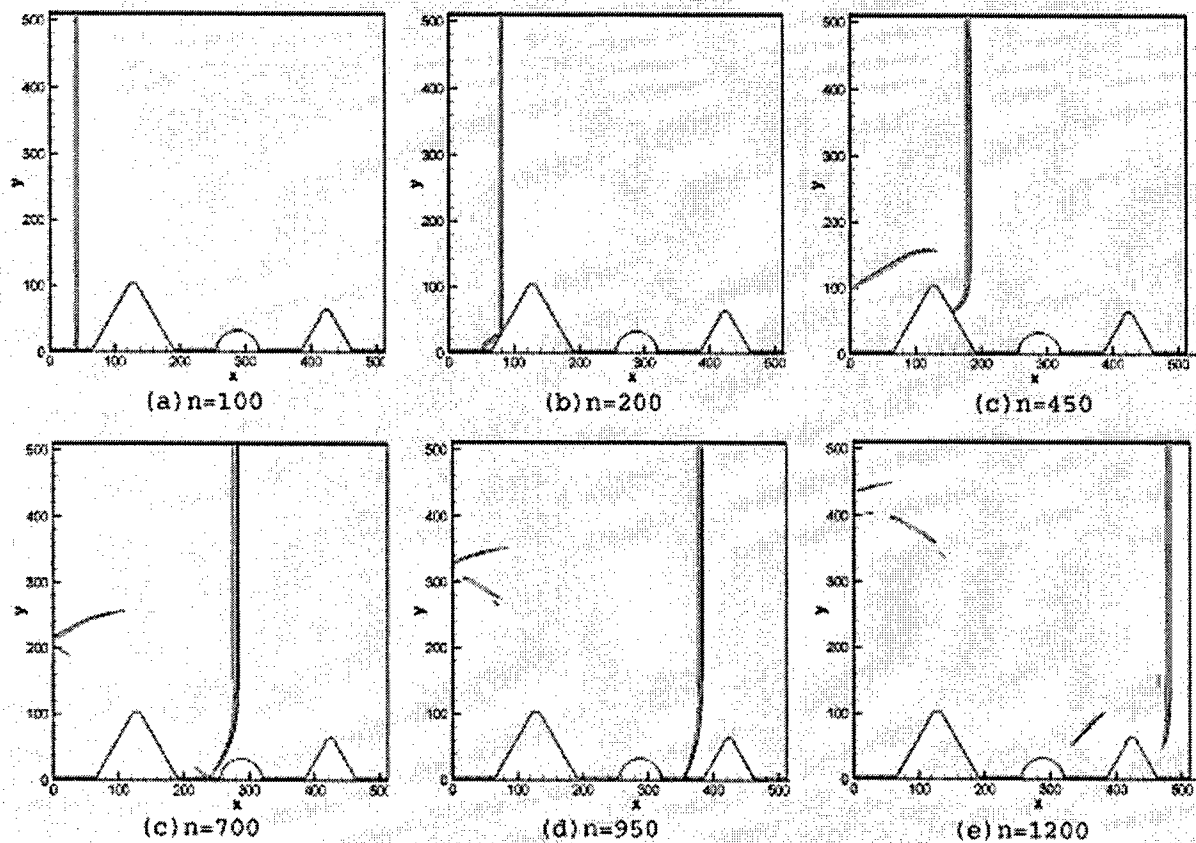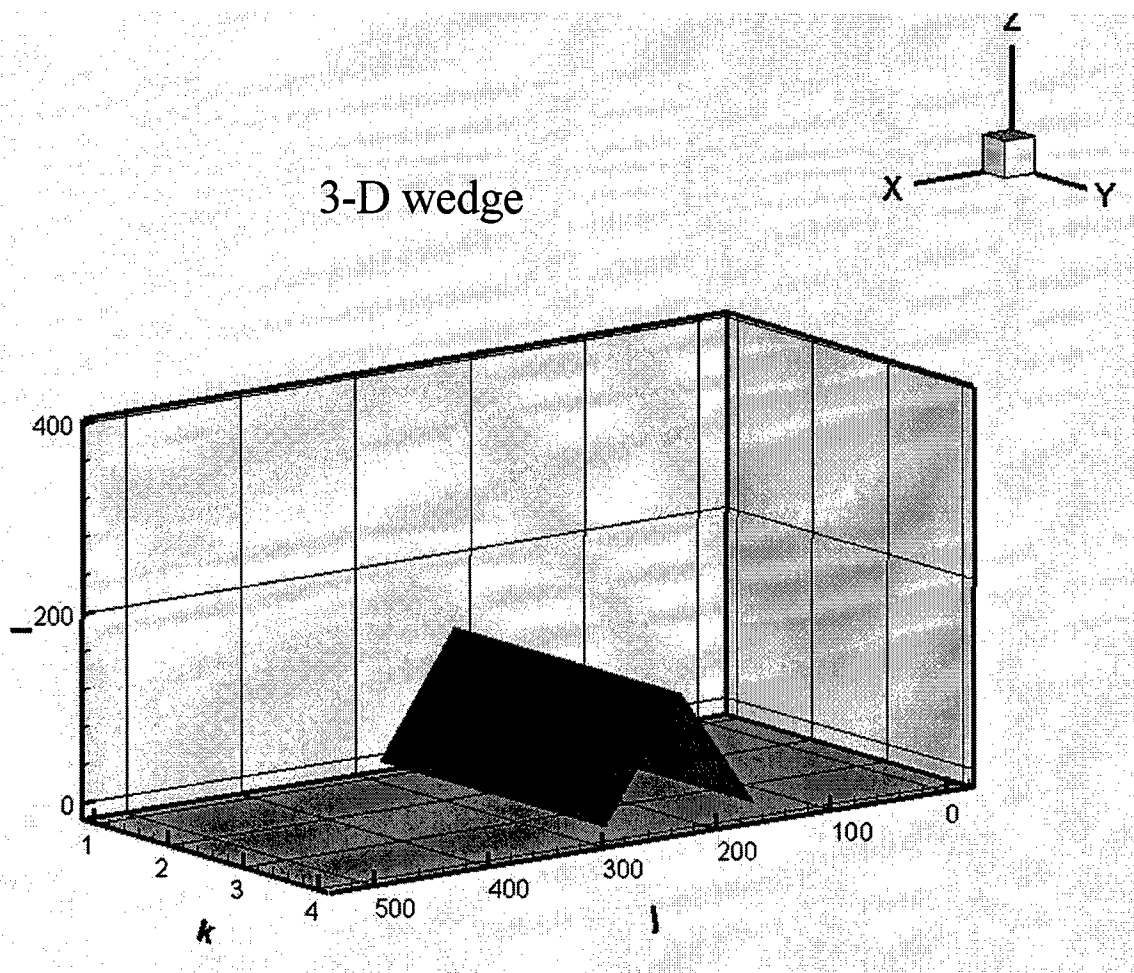Figure 13

Propagating Pulse Amplitude

2-D Terrain

(a)n=100   (b)n=200   (c)n=450

(c)n=700   (d)n=950   (e)n=1200

Figure 14

Figure 15

Pulse Amplitude 3-D Wedge (Eikonal)

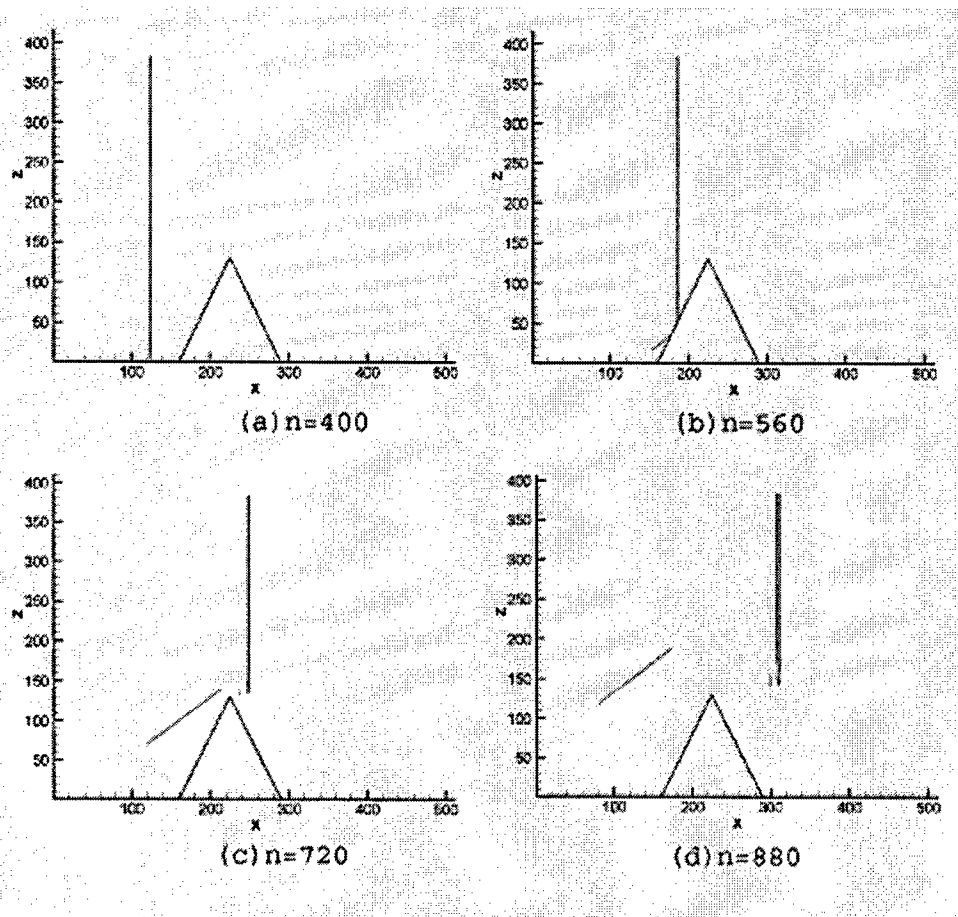(a) n=400   (b) n=560   (c) n=720   (d) n=880

Figure 16

Frequency Domain Phase
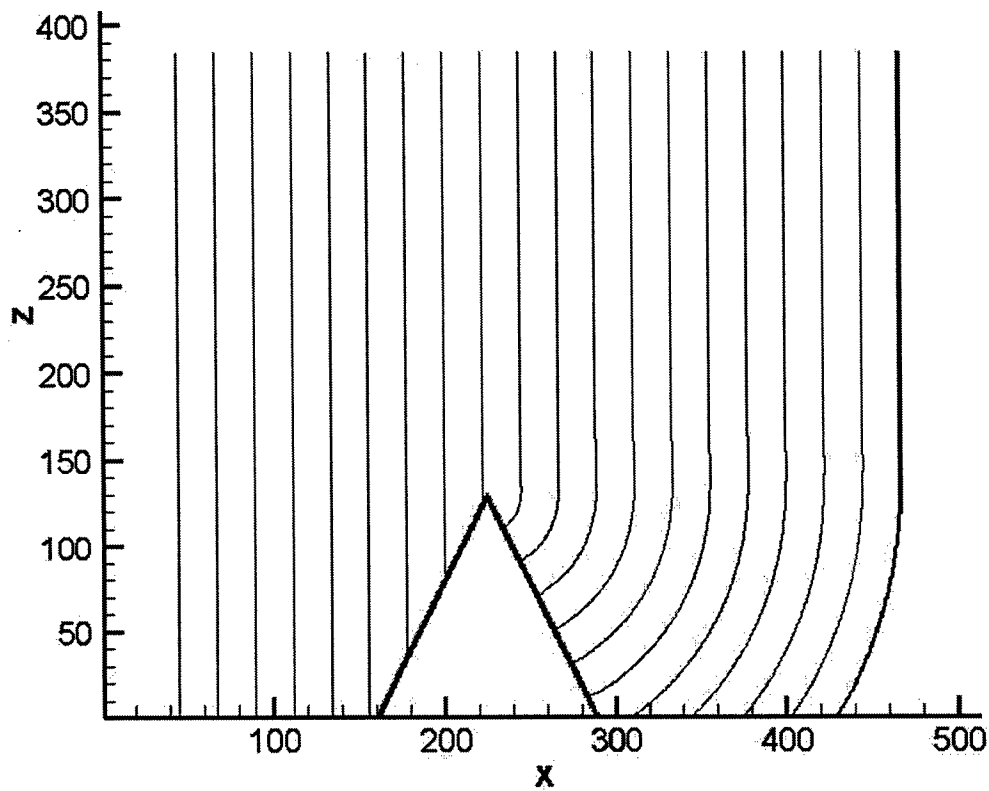# First Arrival (Local Parabolic Method)

Figure 17

Frequency Domain Phases
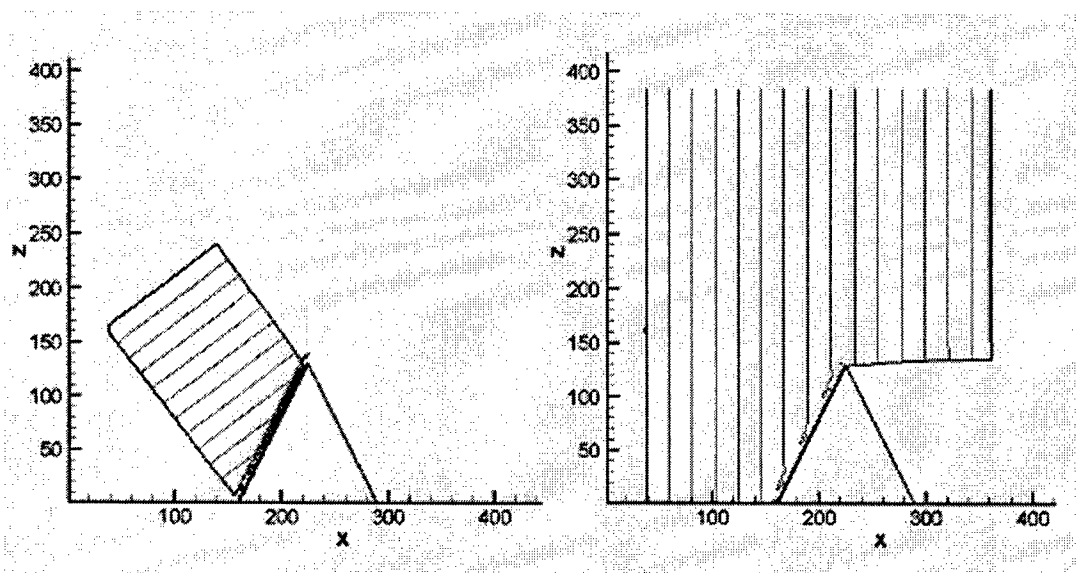## First and Second Arrivals (Eikonal)

Figure 18

Appendix

Computation of Short Wave Equation Pulses Using Nonlinear Solitary Waves

Meng Fan[1], Lesong Wang[2] and John Steinhoff[3]

Abstract A new method is described that has the potential to greatly extend the range of application of current Eulerian time domain electromagnetic or acoustic computational methods for certain problems.

The method involves adding a simple, nonlinear term to the discretized wave equation. As such, it does not require major restructuring of methods or codes that have already been developed. Researchers and engineers who are solving problems for scattering or propagation of short pulses should be able to use the new technique, in many cases as a simple "add on" or callable subroutine, to allow the propagation of short pulses over long distances, even if their solver is low order and the grid is coarse compared to the pulse width (which it must be if the distances are large). The method has many of the advantages of Green's Function based integral equation schemes for long distance propagation. However, unlike these schemes, since it is an Eulerian finite difference technique, it allows short pulses to automatically propagate through regions of varying index of refraction and undergo multiple scattering.

The new method, " Confinement", is based on an earlier, very successful technique, " Vorticity Confinement", that can also be thought of an "add on", which allows the propagation of thin, concentrated vortices over arbitrarily long distances, yet keeps the Eulerian finite difference property of the original fluid dynamic solution method.

In the paper the application of Confinement to the scalar wave equation in 1, 2 & 3 dimensions, including scattering will be described.

keywords: Numerical analysis, wave equation, computational acoustics, computational electromagnetics.

1 Introduction

There are many important problems where thin, concentrated pulses must be numerically convected over long distances. Examples include acoustic and EM pulses scattered or produced by aircraft, rotorcraft and submarines. Often, for these cases, the main interest is in the far field, where the integrated amplitude through the pulse at each point along the pulse surface and the motion of the centroid surface are important, rather than the details of the internal structure. In general, these pulse surfaces can originate in many places, multiply scatter, propagate through varying index of refraction, and have complex topology. Accordingly, we consider Eulerian methods where very general topologies can be treated.

Within this scope, there have been many efforts over decades to discretize and solve the time dependent wave equations. Elaborate codes have been developed to treat complex geometries, such as entire aircraft (we have in mind codes developed by M. Visbal of WPAFB, V. Shankar of Hypercomp Inc. and others). The application of these is, of course, limited by the requirement that sufficient number of grid cells must span the pulse to accurately solve the equations.

A new method has been developed that has the potential to greatly extend the range of application of these computational methods for certain problems. The goal of this effort is that researchers and engineers who are solving problems for scattering or propagation of pulses should be able to use the new technique, in many cases as a simple "add on" or callable subroutine, to allow the propagation of short pulses over long distances, even if their solver is low order and the grid is coarse compared to the pulse width (which it must be if the distances are large). The new method has many of the advantages of

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Green's Function based integral equation schemes for long distance propagation. However, unlike these schemes, since it is an Eulerian finite difference technique, it allows short pulses to automatically propagate through regions of varying index of refraction and undergo multiple scattering.

The new method, " Confinement", is based on an earlier, very successful technique, " Vorticity Confinement", that can also be thought of as an "add on", and which allows the propagation of thin, concentrated vortices over arbitrarily long distances, yet keeps the Eulerian finite difference property of the original fluid dynamic solution method.

Confinement involves treating a thin feature, such as a pulse, as a type of weak solution of the governing partial differential equation (pde). Within the feature, a nonlinear *difference* equation, as opposed to *finite difference* equation, is solved that does not necessarily represent a Taylor expansion discretization of the pde. The approach is similar to shock capturing [Lax(1957)], where conservation laws are satisfied, so that integral quantities such as total amplitude and centroid motion are accurately computed for the feature. A more general approach is needed, however, than for shocks, as discussed below. Basically, we treat the features as multi-dimensional nonlinear discrete solitary waves that " live" on the computational lattice. These obey a "confinement" relation that is a generalization to multiple dimensions of some earlier 1-D contact discontinuity capturing schemes.

Differences between Confinement and conventional 1-D shock capturing, are that:

First, unlike shocks, characteristics do not point into the feature, and extra terms must be designed to prevent it from spreading due to numerical effects in the convection. (Harten [Harten(1978)] developed such a scheme, but for contact discontinuities in 1-D compressible flow.)

Second, thin wave equation pulses, vortex filaments or thin streams of passive scalars, are intrinsically multi-dimensional: A concatenation of 1-D " capturing" operators along separate axes will not, generally, give smooth solutions. Due to the multidimensional nature, it seems necessary to pay some attention to the (modeled) structure within the feature, even though it is sampled on only a few grid cells in the cross-section.

First, a short critique of conventional methods for these problems is given. The basic new method is then described. Initial results in 1, 2 & 3D are finally presented.

The method presented has a similar goal to that of [Bleszynski, Bleszynski and Jaroszewicz (2004)] in that they propagate a continuous wave surface in the high frequency limit. The main difference is that they use a system of coupled rays and we use an Eulerian approach.

Also, they are already treating diffractive effects, which we are now starting to do.

2 Current Methods

Conventional Eulerian approaches to the wave equation problem involve, of course, formulating governing pde's, discretizing them and solving them as accurately as possible on feasible computational grids, assuming smooth enough solutions. For smooth, non-thin pulses, these methods are well known to converge to the correct solution as the number of points across the pulse, N, becomes large: Error estimates are asymptotic in N. For accurate solutions, even higher order, complex discretization methods typically require N to be at least ~8 or 10 so that the error obeys the large N estimate and is small [Visbal and Gaitonde (1998)]. Even then, solutions degrade over long convection distances (thousands of pulse widths). As a result, conventional methods may be inefficient (or not even feasible) for thin pulses convecting over long distances. Further, adaptive, unstructured grids cannot improve the resolution significantly for realistic problems with many thin, time dependent pulse surfaces.

3 Confinement Approach

3.1 Basic Features

For the above reasons, for the problems considered, it is important to have only very few (2 or 3) grid points to represent the cross section of a pulse surface at each point along the surface and to propagate it with no numerical spreading. This small number of grid points is consistent with the desire to only compute a few integral quantities across the pulse, such as total amplitude and centroid position, and perhaps width or a small number of moments. Then, the difference scheme can, effectively, serve as a simple, implicit "solitary wave" model that *represents* the wave.

An important point is that both the solitary wave pulse thickness and the physical pulse thickness (they may be different) are assumed to be small compared to the other scales in the region where the method is used. Thus, the pulse propagates according to geometrical optics (high frequency limit) in the region.

The basic idea is that we want to propagate the minimum amount of information necessary to describe the pulse. When it is thick, compared to other dimensions, such as the nearby details of the scatterer, we may choose to use a fine grid and represent the full physical pulse profile. As it propagates away, we may just be interested, as explained, in integral quantities at each point along the

pulse surface, i.e., along a ray normal to the surface. As the pulse propagates away, we may have to use a coarser grid that may even have cells larger than the physical pulse thickness, while retaining this information in our "representative" solitary wave.

An important point is that, when the pulse thickness is much less than the radius of curvature of the pulse surface, it is more efficient to describe the pulse profile by a number of "moment fields". The resolution of the thickness profile then depends linearly on the number of these moment fields, which only increases linearly with the resolution. This is then also true of computational storage and work requirements. This should be contrasted with conventional discrete Eulerian schemes, where the cell size is determined by the required resolution. There, for general configurations of surfaces, the number of grid nodes (and computer storage) in 3-D increases like the third power of the resolution and, (including time step changes), the work increases like the fourth power.

As explained in the next section, when the grid is coarse, the Confinement method allows pulse surfaces to propagate over arbitrarily long distances while treating them as nonlinear solitary waves, spread over ~ 2 grid cells, thus allowing information to be accurately propagated. On the other hand, when the grid is fine and details need to be resolved, the Confinement terms automatically become small and the method can automatically become conventional computational acoustics (or electromagnetics). Further, if a pulse propagates through a smooth medium as a solitary wave and then encounters a scatterer where details must be resolved, the pulse can be "reconstituted" on the (new) fine grid, if enough moments are available. This reconstitution will require a "pulse shaping" step. This can easily be effected since, in addition to the common positive numerical diffusion, with confinement, we have a stable *total* negative diffusion, as explained below. Thus, the fine grid pulse can be expanded or contracted until its moments agree with the correct values (this is a subject of current work). This feature will be important in many cases, for example, when a pulse scatters from an aircraft wing, propagates many pulse widths, and scatters again from a tail where fine details must be resolved. Further, multiple scattering in inlets for short pulses should provide an important application.

3.2 Approach

The governing equation discussed here is the discretized scalar wave equation, with an added Confinement term: (the approach also works for vectors or tensors, such as Maxwell's equations.)

$$\partial_t^2 \phi = \sigma^2 \nabla^2 \phi + \frac{h^2}{\Delta t}\nabla^2[\mu\phi - \varepsilon\Phi]$$

(1)

where ϕ is the scalar amplitude, σ is the index of refraction, μ is a diffusion coefficient that includes numerical effects (we assume physical diffusion is much smaller), and the discretized grid cell size is h and time step, Δt. For the last term, $\varepsilon\Phi$, ε is a numerical coefficient that, together with μ, controls the thickness and time scales of the propagating pulse. Φ will be defined below. For this reason, we refer to the two terms in the brackets as "Confinement terms". We assume conventional, not necessarily high order discretizations are used for the differential operators.

We have found that, at least in tests involving propagation through regions of constant index refraction, the results are similar, to plottable accuracy, whether or not the time derivative is included on the RHS of Eq. (1). However, since the time derivative enforces a relaxation to the desired pulse shape (as explained below), we believe it should be included in general.

The basic idea is that we want the computed thin pulses to maintain their profile and total amplitude as their centroid surfaces are propagated through the field. (We want the same for separate pulse fields representing moments.) The requirement that they relax to their profile in a small number of time steps and have a support of a small number of grid cells determines the two parameters, ε and μ. Also, we assume that the index of refraction field in which the pulse is propagating is slowly varying in time and space compared to these scales (this is required anyway if the grid cell size and time step are to resolve this field). We then have a two-scale problem with the thin pulse obeying a "fast" dynamics.

$$\nabla^2(\mu\phi - \varepsilon\Phi) \approx 0,$$

(2)

Thin pulses are then propagated through the field by the "slow" variable, σ. Exactly the same type of discussion applies to the convection of passive scalars, as described in Ref. [Steinhoff, Fan, Wang and Dietz (2003)].

In general, the integrals that we are interested in are not sensitive to the parameters ε and μ over a wide range of values, as long as the computed pulses are thin.

An important feature of the Confinement method is that, since it is a second derivative in space and first in time, the total amplitude and centroid of the surface are not changed by the added confinement terms, even under discretization.

3.3 Formulation

The formulation for Confinement will first be described for a stationary pulse, for clarity. The scalar formulation presented here is related to that presented in [Steinhoff, Wenren, Underhill and Puskas (1995), Steinhoff, Puskas, Babu, Wenren and Underhill (1997)] in 1-D. This " fast" dynamics will be realized in a wave equation computation in the limit of small time step, or if a separate " Confinement" iteration is done each time step. Excellent results are found with convection and are shown in [Steinhoff, Fan, Wang and Dietz (2003)] for vorticity as well as convecting passive scalars.

For this case, we have an iteration for a non-negative scalar, ϕ:

$$\phi^{n+1} = \phi^n + \mu h^2 \nabla^2 \phi^n - \varepsilon h^2 \nabla^2 \Phi^n$$

(3)

where

$$\Phi^n = \left[\frac{\sum_l C_l (\tilde{\phi}^n)^{-1}}{\sum_l C_l} \right]^{-1}$$

(4)

$$\tilde{\phi}^n = |\phi|^n + \delta$$

(5)

where the sum is over a set of grid nodes near and including the node where Φ is computed, the absolute value is taken and δ, a small positive constant ($\sim 10^{-8}$) is added to prevent problems due to finite precision. The coefficients, C_l, can depend on l, but good results are obtained by simply setting them all to 1 for the wave equation (different values are used for passive scalar convection to avoid using downwind values [Steinhoff, Fan, Wang and Dietz (2003)]. Eq. (4) is related to the harmonic mean.

For example, in 2D, except for convecting scalars, the form used in this study is

$$\Phi_{ij}^n = \left[\frac{\sum_{\alpha=-1}^{+1} \sum_{\beta=-1}^{+1} (\tilde{\phi}_{i+\alpha, j+\beta}^n)^{-1}}{N} \right]^{-1}$$

(6)

where the number of terms in the sum is N=9. Here, we assume $\phi^n \geq 0$. Negative values can also be accommodated with a small extension. Both μ and ε are positive.

An important feature is that all terms are homogeneous of degree 1 in Eq. (4). This is important because the confinement should not depend on the scale of the quantity being confined. Another important feature is the nonlinearity. It is easy to show that a linear combination of terms, for example of second and fourth order, cannot lead to a stable confinement for any finite range of coefficients.

For smooth ϕ fields (long wavelengths), the last term in Eq. (1) represents a diffusion. If $\mu \leq \varepsilon$, the total diffusion (in the long wavelength limit) is negative. However, the iteration of Eq. (3) is still stable and has been observed to converge for values of ε several times that of μ (depending on value of μ).

3.4 Analysis of Small Time Step Form

(Sections 3.4 and 3.5 are close to part of Ref. [Steinhoff, Fan, Wang and Dietz (2003)].

Stability of the iteration as $n \to \infty$ can easily be shown [Steinhoff and Lynn (2002)] for a range of values of μ and ε, including $\mu \leq \varepsilon$. We only have to start with a non-negative initial (ϕ^0) field and show that, for the μ and ε values, ϕ^n remains non-negative. Since the sum of ϕ values is conserved, there is thus an upper bound. Assuming convergence as $n \to \infty$, we have

$$\nabla^2 (\mu \phi - \varepsilon \Phi) = 0$$

(7)

If ϕ (and hence Φ) vanishes in the far field, away from the pulse, we have $\mu \phi = \varepsilon \Phi$,

If the point (i, j) is given the label $l = 0$, we then have

$$\phi_0^{-1} - \frac{\mu}{\varepsilon N} \sum_l \phi_l^{-1} = 0$$

(8)

There are many solutions of this equation. The ones of importance to us are of the form

$$\phi_{ij} = A \sec h[\alpha(z - z_0)]$$

(9)

$$z = x_i \cos \theta + y_j \sin \theta$$

(10)

A, α, z_0, θ constant, and where $x_i = ih$, $y_j = jh$, h is the grid cell size, and we use the form corresponding to $C_l = 1$ in Eq. (4). This converges to a straight pulse (in 2-D) concentrated about a line at angle θ. It is easy to see that α satisfies

$$\frac{\varepsilon}{\mu} = [1 + 2ch(\alpha h \cos\theta) + 2ch(\alpha h \sin\theta)]/5$$
(11)

for $N = 5$.

An important point is that we obtain close to the same invariance properties as the original pde: The solution is translationally invariant (z_0 is arbitrary) and close to rotationally invariant (θ is arbitrary with a width, given by α in Eq.(11), having some dependence on θ).

3.5 Convection of Passive Scalar

Since the wave equation is, of course, closely related to the convection equation, we present some analysis for the latter, since it is simpler. This analysis shows that the pulse convects with the weighted mean velocity, where the pulse amplitude is the weight. This " Ehrenfest" type of relation should extend to the full wave equation.

The following argument assumes, for each convection step (n), there is at least one confinement step so that the feature remains compact. If ϕ represents a confined passive scalar, then, using a conservative convection routine, we have the following relationships for the dynamics of the convecting solitary wave (we describe the 2-D case for simplicity):

We have a discretization of

$$\partial_t \phi = -\bar{\nabla} \cdot (\vec{q}\phi) + h^2 \nabla^2 (\mu\phi - \varepsilon\Phi)/\Delta t$$
(12)

assuming $\bar{\nabla} \cdot \vec{q} = 0$. Then,

$$\phi^{n+1} = \phi^n - \Delta t \bar{\nabla}_{disc} \cdot (\vec{q}\phi) + h^2 \nabla^2_{disc}(\mu\phi - \varepsilon\Phi)$$
(13)

where discrete operators are labeled.

For conservative discretization, the total amplitude

$$\Omega \equiv \sum_{ij} \phi_{ij}^n$$
(14)

is independent of n. If we define the centroid

$$<\vec{X}>^n \equiv \sum_{ij} \vec{x}_{ij}\phi_{ij}^n / \Omega$$
(15)

and the weighted mean velocity

$$<\vec{q}>^n \equiv \sum_{ij} \vec{q}_{ij}^n \phi_{ij}^n / \Omega$$
(16)

where $\vec{x}_{ij}$ is the (fixed) position vector of node (i, j), and ϕ_{ij} and $\vec{q}_{ij}$ are the scalar value and the velocity at that node, then the centroid evolves according to:

$$<\vec{X}>^{n+1} = <\vec{X}>^n + \Delta t <\vec{q}>^n$$
(17)

Since we are, at this point, only interested in the "expectation values" for thin pulses and that the pulses remain compact, spread over only a few cells, this Ehrenfest-type relation is exactly what we need. Only the variables of importance are, effectively, solved for. This shows that the pulses, when isolated, evolve as surfaces with essentially no internal dynamics (assuming they remain confined as thin surfaces). However, we keep the very important Eulerian feature that the number of pulses is not fixed. We could, for example, create additional solitary waves by inserting a source: No additional computational markers need be created, as in Lagrangian schemes. For this study, we show that pulses, for example, reflect and thereby increase automatically in number. This will be seen in the results of Sec. 4.

4 Results

For the scalar wave equation, a simple second-order centered difference method was used for the discretization of Eq. (1). We solve it through two steps: the first is a conventional wave equation solver step, and the second is the confinement step

$$\phi^* = 2\phi^n - \phi^{n-1} + \sigma^2(\Delta t)^2 \nabla^2_{disc.}\phi^n$$
(18)

$$\phi^{n+1} = \phi^* + h^2 \nabla^2_{disc.}\delta_n^-(\mu\phi^* - \varepsilon\Phi^*)$$
(19)

where $\nabla^2_{disc.}$ and δ_n^- are the second-order centered difference approximation for the Laplace ∇^2 operator and the backward difference operator in n.

For the 1-D and 2-D result plots, axes are labeled with grid node location. For the 2-D and 3-D results, plots of amplitude are made using dense contours.

4.1 1-D Wave Equation

We start a single pulse in the center of a 256 cell grid with periodic boundary conditions. This pulse has an initial amplitude of 2 at the single, central grid point and is zero at all other points. The resulting two opposite moving waves are shown in Fig. 1 for no Confinement (1a) and Confinement (1b). A minimal diffusion necessary for stability, $\mu = 0.025$, with $\varepsilon = 0$ was used in 1a while in 1b $\mu = 0.1$, $\varepsilon = 0.8$. The rapid diffusion can be seen in 1a, while in 1b the bulk of the pulses remain confined to ~3 grid cells and have no diffusion. Other tests show that they continue unaltered for up to about 10^6 time steps, and beyond if double precision is used. This was also shown with an earlier Confinement form in Ref. [Steinhoff, Wenren, Underhill and Puskas (1995)].

It should be noted that even though the Confinement is nonlinear, there is virtually no interaction when the waves pass through each other. This was shown in detail in Ref. [Steinhoff, Wenren, Underhill and Puskas (1995)].
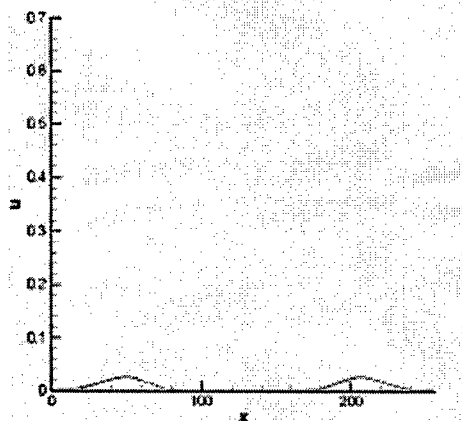
(a) fifteenth pass
(no Confinement)
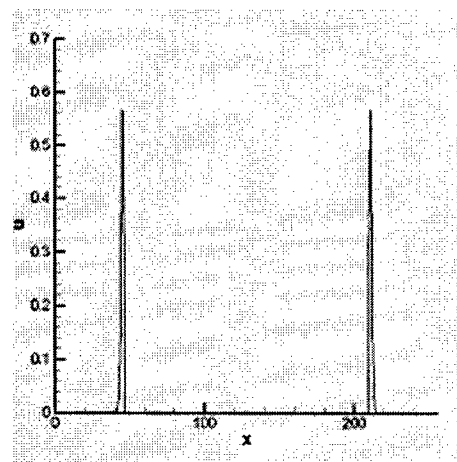
(b) fifteenth pass
(with Confinement)

Figure 1: 1D pulse propagation

4.2 2-D Wave Propagation

Waves were propagated on a $(128)^2$ cell grid with reflecting boundary conditions. Confinement values used were $\mu = 0.08$, $\varepsilon = 0.6$. Of course, the actual wave equation exhibits a "tail" behind a pulse in 2-D. This can be seen to be suppressed by the Confinement, and, effectively, only the steep pulse front is accurately computed. The tail, since it is smooth, could be computed with no Confinement. The main interest, however, is in 3-D and this was not done.

4.2.1 Convex Wave

An outward propagating, initially circular pulse surface (diameter 64 cells) was computed. It can be seen in Fig.2 that it remains sharply confined, even after many reflections. Again, as in 1-D, there is no discernable interaction between intersecting waves.

4.2.1 Concave and Convex Waves

The same computation was done as in 4.2.1, but with an initially 2:1 elliptical surface, with 64 cell major axis. Both inward and outward moving waves were formed. The inward moving wave can be seen to form cusps and "swallowtails" . These are only initially resolved, because of the coarseness of the grid. The basic discrete wave equation method, without Confinement, would, of course, not do better. It is well known that refinement is needed in such regions for direct application of finite difference schemes [Benamou and Solliec (2000)].

4.3 3-D Convex Wave Propagation

An expanding, initially spherical pulse surface was computed on a coarse, $(64)^3$ cell grid with reflecting boundary conditions. The initial diameter was 32 cells. Confinement values used were $\mu = 0.05$ and $\varepsilon = 0.4$. As in the 2-D case, the pulse remains completely confined, even after many reflections.
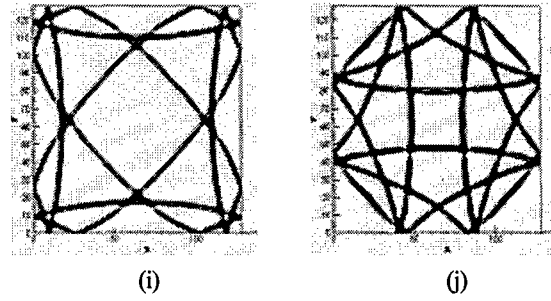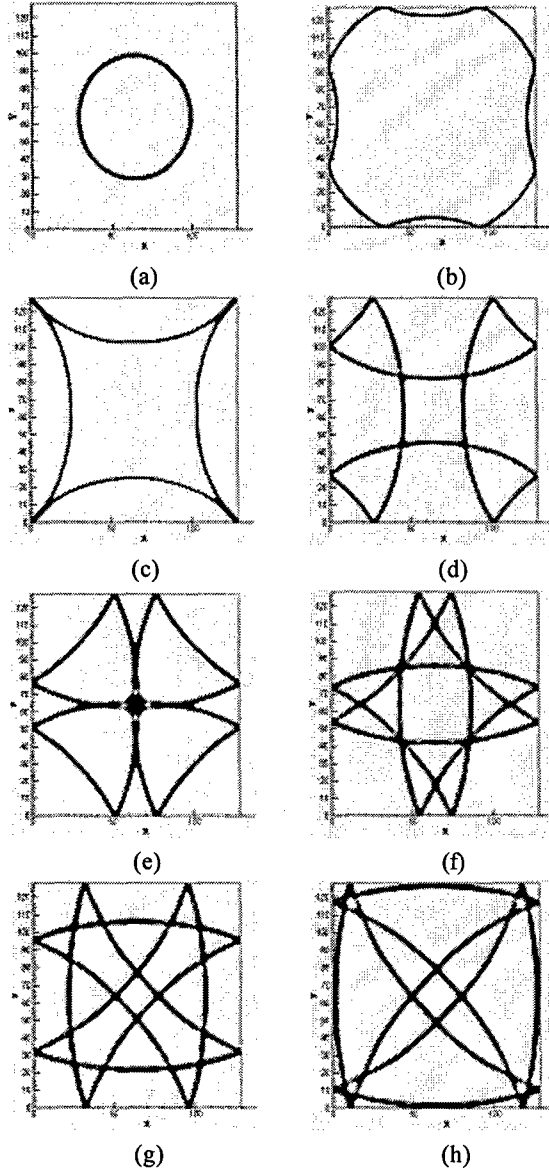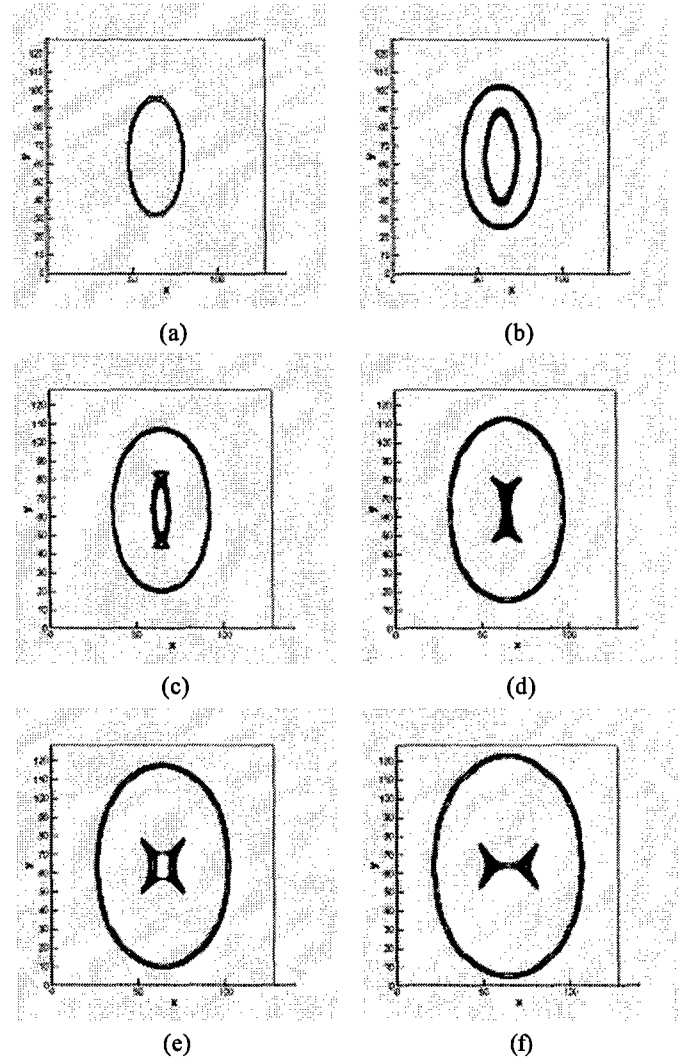

(a)

(b)

(c)

(d)

(e)

(f)

(g)

(h)

(i)

(j)

Figure 2: 2D circle wave propagation

(a)

(b)

(c)

(d)

(e)

(f)

Figure 3: 2D convex and concave wave propagation: Cusp Formulation

5   Conclusion

(e)   (f)

Figure 4: 3D convex wave propagation

A new Eulerian technique is introduced for solving the wave equation for short pulses. The method, " Confinement" , reduces to standard Eulerian ones for smooth, long wavelength pulses. However, unlike conventional schemes, it does not diffuse short pulses. Instead, they are " Confined" and propagate as nonlinear solitary waves that " live" on the computational lattice. As such, they can be propagated over indefinitely long distances, while remaining only 2~3 cells thick. These pulses *represent* the short physical pulses and accurately propagate integral quantities at each point along the pulse surface, such as total amplitude, centroid position, pulse width and other desired moments. It is argued that, for thin pulses, the method can easily be implemented in existing codes, allowing them to be extended to treat much higher wavelengths/shorter pulses, without extensive reformulation. Examples are shown in 1-D, 2-D and 3-D.

6   Acknowledgements

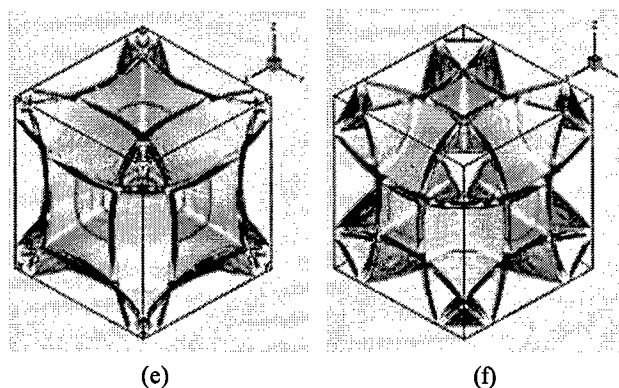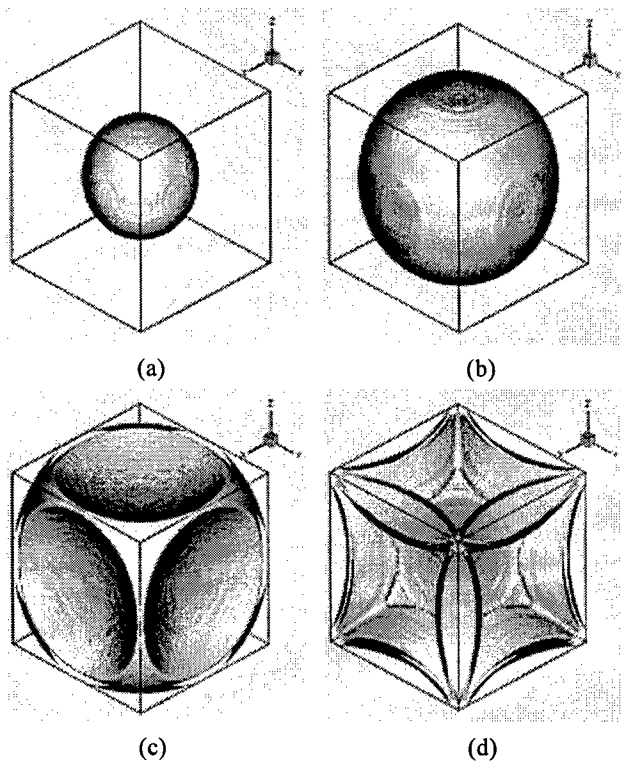(a)   (b)

(c)   (d)

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